ELSEVIER

Chemical Physics 270 (2001) 483–487

Chemical Physics

www.elsevier.com/locate/chemphys

# Author Index

Bai, J., see Hua, X. 270 (2001) 93
Barvík, I., see Čápek, V. 270 (2001) 141
Bhattacharyya, S.P., see Chaudhury, P. 270 (2001) 277
Billard, I., A. Rustenholtz, L. Sémon and K. Lützenkirchen, Fluorescence of $UO_2^{2+}$ in a non-complexing medium: $HClO_4/NaClO_4$ up to 10 M 270 (2001) 345
Børve, K.J., see Karlsen, T. 270 (2001) 55
Brion, C.E., G. Cooper, Y. Zheng, I.V. Litvinyuk and I.E. McCarthy, Imaging of orbital electron densities by electron momentum spectroscopy – a chemical interpretation of the binary (e,2e) reaction 270 (2001) 13
Brion, C.E., see Feng, R. 270 (2001) 319
Brion, C.E., see Tixier, S. 270 (2001) 263

Čápek, V., I. Barvík and P. Heřman, Towards proper parametrization in the exciton transfer and relaxation problem: dimer 270 (2001) 141
Carlos del Valle, J., and J. Catalán, Understanding the solvatochromism of 10-hydroxybenzo[h]quinoline. An appraisal of a polarity calibrator 270 (2001) 1
Catalán, J., see Carlos del Valle, J. 270 (2001) 1
Češljević, V.I., see Szabó, A. 270 (2001) 67
Chaudhury, P., R. Saha and S.P. Bhattacharyya, Structure and vibrational spectroscopy of halide ion hydrates: a study based on genetic algorithm 270 (2001) 277
Chen, M.C., C.R. Lambert, J.D. Urgitis and M. Zimmer, Photoisomerization of green fluorescent protein and the dimensions of the chromophore cavity 270 (2001) 157
Chen, Y., see Chen, Z.-X. 270 (2001) 253
Chen, Z.-X., C.-G. Liu, Y. Chen and Y.-S. Jiang, Theoretical investigation on $BaTiO_3$ with periodic density functional theory BLYP method 270 (2001) 253
Chikhaoui, A., see Kustova, E.V. 270 (2001) 459
Chong, D.P., see Tixier, S. 270 (2001) 263
Cooper, G., see Brion, C.E. 270 (2001) 13
Cooper, G., see Feng, R. 270 (2001) 319
Cooper, L., L.G. Shpinkova, D.M.P. Holland and D.A. Shaw, A study of the threshold photoelectron spectra and the photoionisation yield curves of the silicon tetrahalides 270 (2001) 363

Dimicoli, I., see Piuzzi, F. 270 (2001) 205
Dong, S., Y. Wang and J. Li, Potential lattice dynamical simulations of ice 270 (2001) 309

PII: S0301-0104(01)00435-9

Farnan, I., see Kristensen, J.H. 270 (2001) 109
Feng, R., G. Cooper and C.E. Brion, Ionic photofragmentation and photoionization of dimethyl ether in the VUV and soft X-ray regions (8.5–80 eV) – absolute oscillator strengths for molecular and dissociative photoionization 270 (2001) 319
Flemmig, B., H. Modrow, K.H. Hallmeier, J. Hormes, J. Reinhold and R. Szargan, Sulfur in different chemical surroundings – S K XANES spectra of sulfur-containing heterocycles and their quantum-chemically supported interpretation 270 (2001) 405
Fukuchi, T., see Iwahashi, K. 270 (2001) 333
Furusawa, J., see Iwahashi, K. 270 (2001) 333

Galasso, V., On the structure and spectroscopic properties of free and protonated adamanzanes 270 (2001) 79
Gastilovich, E.A., V.G. Klimenko, N.V. Korol'kova and G. Rauhut, Excited electronic states and effect of vibronic-spin–orbit coupling on the radiative deactivation of the lowest triplet states of dioxins 270 (2001) 41
Grachev, A.V., see Ronova, I.A. 270 (2001) 99
Gusev, A.I., see Makurin, Yu.N. 270 (2001) 293

Hallmeier, K.H., see Flemmig, B. 270 (2001) 405
Heřman, P., see Čápek, V. 270 (2001) 141
Holland, D.M.P., see Cooper, L. 270 (2001) 363
Hormes, J., see Flemmig, B. 270 (2001) 405
Hua, X., J. Bai and L. Wang, "Plasma" effect in the formation of long lifetime Rydberg states 270 (2001) 93

Imhof, P. and K. Kleinermanns, Dispersed fluorescence spectra of chlorobenzene 270 (2001) 227
Ivanovsky, A.L., see Makurin, Yu.N. 270 (2001) 293
Iwahashi, K., N. Yamamoto, T. Fukuchi, J. Furusawa and H. Sekiya, Hole-burning spectra of tropolone–$(CO_2)_n$ $(n = 1, 2)$ van der Waals complexes and density functional study 270 (2001) 333

Jiang, Y.-S., see Chen, Z.-X. 270 (2001) 253
Joarder, R.N., see Sarkar, S. 270 (2001) 197
Johansson, A., see Ubachs, W. 270 (2001) 215
Jovanović-Kurepa, J., see Terzić, M. 270 (2001) 383
Ju, G., see Wei, J. 270 (2001) 31
Jung, K.-H., see Park, M.S. 270 (2001) 133

Karlsen, T., K.J. Børve and L.J. Sæthre, Second-order Møller–Plesset perturbation theory for computing molecular-field splitting: application to the $S2p_{3/2}$ level in $C_2H_{2n+1}SF_5$, $n = 0$, 1, and 2 270 (2001) 55
Kleinermanns, K., see Imhof, P. 270 (2001) 227
Klimenko, V.G., see Gastilovich, E.A. 270 (2001) 41
Korol'kova, N.V., see Gastilovich, E.A. 270 (2001) 41
Koutselos, A.D., Third-order transport properties of ions in electrostatic fields 270 (2001) 165
Kovács, A., see Szabó, A. 270 (2001) 67
Kovalevsky, A.Yu., see Ronova, I.A. 270 (2001) 99

Kristensen, J.H. and I. Farnan, Computational aspects of motional symmetry in nuclear magnetic resonance spectroscopy 270 (2001) 109
Kück, S., see Sokólska, I. 270 (2001) 355
Kustova, E.V., On the simplified state-to-state transport coefficients 270 (2001) 177
Kustova, E.V., E.A. Nagnibeda and A. Chikhaoui, On the accuracy of non-equilibrium transport coefficients calculation 270 (2001) 459

Lambert, C.R., see Chen, M.C. 270 (2001) 157
Lang, R., see Ubachs, W. 270 (2001) 215
Lemarchand, A., see Nowakowski, B. 270 (2001) 287
Levine, R.D., On the capture cross-section for charge neutralization, recombination, photoassociation and other barrierless reactions 270 (2001) 129
Li, J., see Dong, S. 270 (2001) 309
Li, Z.S., see Ubachs, W. 270 (2001) 215
Litvinyuk, I.V., see Brion, C.E. 270 (2001) 13
Liu, C.-G., see Chen, Z.-X. 270 (2001) 253
Lokhnygin, V., see Ubachs, W. 270 (2001) 215
Lu, Y., see Xie, D. 270 (2001) 415
Lützenkirchen, K., see Billard, I. 270 (2001) 345

Makurin, Yu.N., A.A. Sofronov, A.I. Gusev and A.L. Ivanovsky, Electronic structure and chemical stabilization of $C_{28}$ fullerene 270 (2001) 293
Malakhovskii, A.V., Ejection of cluster ions as a result of electron impact ionization of argon clusters 270 (2001) 471
Markushev, D., see Terzić, M. 270 (2001) 383
McCarthy, I.E., see Brion, C.E. 270 (2001) 13
Messmer, R.P., see Sejpal, M. 270 (2001) 237
Modrow, H., see Flemmig, B. 270 (2001) 405
Molinari, E. and M. Tomellini, Non-equilibrium vibrational kinetics and 'hot atom' models in the recombination of hydrogen atoms on surfaces 270 (2001) 439
Mons, M., see Piuzzi, F. 270 (2001) 205

Nagnibeda, E.A., see Kustova, E.V. 270 (2001) 459
Nath, P.P., see Sarkar, S. 270 (2001) 197
Nowakowska, E., see Nowakowski, B. 270 (2001) 287
Nowakowski, B., A. Lemarchand and E. Nowakowska, Nonstandard reaction kinetics: microscopic simulations of system with product removal 270 (2001) 287

Pandey, J.D. and R. Verma, Inversion of the Kirkwood–Buff theory of solutions: application to binary systems 270 (2001) 429
Park, M.S, K.-H. Jung, H.P. Upadhyaya and H.-R. Volpp, The dynamics of oxygen atom formation in the UV photodissociation of nitromethane 270 (2001) 133
Pickholz, M. and S. Stafström, Theoretical investigation of the role of $\pi$–$\pi$ interactions for the stability of phenylene ethynylene aggregates 270 (2001) 245
Piuzzi, F., M. Mons, I. Dimicoli, B. Tardivel and Q. Zhao, Ultraviolet spectroscopy and tautomerism of the DNA base guanine and its hydrate formed in a supersonic jet 270 (2001) 205

Rauhut, G., see Gastilovich, E.A. 270 (2001) 41
Reinhold, J., see Flemmig, B. 270 (2001) 405
Ronova, I.A., A.Yu. Kovalevsky, S.A. Siling, S.V. Shamshin, A.V. Grachev and O.Yu. Tsyganova, Bifluorophors: molecular design and excitation energy transfer mechanism 270 (2001) 99
Rustenholtz, A., see Billard, I. 270 (2001) 345

Sæthre, L.J., see Karlsen, T. 270 (2001) 55
Saha, R., see Chaudhury, P. 270 (2001) 277
Sarkar, S., P.P. Nath and R.N. Joarder, Orientation correlation of neopentane molecules in liquid state through available diffraction data 270 (2001) 197
Sejpal, M. and R.P. Messmer, On the size extensivity of second-order Møller–Plesset perturbation theory based on a perfectly-paired generalized valence bond reference wavefunction 270 (2001) 237
Sekiya, H., see Iwahashi, K. 270 (2001) 333
Sémon, L., see Billard, I. 270 (2001) 345
Shamshin, S.V., see Ronova, I.A. 270 (2001) 99
Shapley, W.A., see Tixier, S. 270 (2001) 263
Shaw, D.A., see Cooper, L. 270 (2001) 363
Shi, Z., see Tixier, S. 270 (2001) 263
Shpinkova, L.G., see Cooper, L. 270 (2001) 363
Siling, S.A., see Ronova, I.A. 270 (2001) 99
Sofronov, A.A., see Makurin, Yu.N. 270 (2001) 293
Sokólska, I. and S. Kück, Observation of photon cascade emission in the $Pr^{3+}$-doped perovskite $KMgF_3$ 270 (2001) 355
Stafström, S., see Pickholz, M. 270 (2001) 245
Szabó, A., V.I. Češljević and A. Kovács, Tautomerism, hydrogen bonding and vibrational properties of 4-acetyl-3(5)-amino-5(3)-methylpyrazole 270 (2001) 67
Szargan, R., see Flemmig, B. 270 (2001) 405

Tardivel, B., see Piuzzi, F. 270 (2001) 205
Tchang-Brillet, W.-Ü.L., see Ubachs, W. 270 (2001) 215
Terzić, M., D. Markushev and J. Jovanović-Kurepa, Bulk rotational relaxation time and cross-section in gas mixtures 270 (2001) 383
Tixier, S., W.A. Shapley, Y. Zheng, D.P. Chong, C.E. Brion, Z. Shi and S. Wolfe, Electron densities for the outer valence orbitals of pyridine: comparison of EMS measurements with near Hartree–Fock limit and density functional theory calculations 270 (2001) 263
Tomellini, M., see Molinari, E. 270 (2001) 439
Tsyganova, O.Yu., see Ronova, I.A. 270 (2001) 99

Ubachs, W., R. Lang, I. Velchev, W.-Ü.L. Tchang-Brillet, A. Johansson, Z.S. Li, V. Lokhnygin and C.-G. Wahlström, Lifetime measurements on the $c_4'^1\Sigma_u^+$, $v = 0$, 1 and 2 states of molecular nitrogen 270 (2001) 215
Upadhyaya, H.P., see Park, M.S. 270 (2001) 133
Urgitis, J.D., see Chen, M.C. 270 (2001) 157

Velchev, I., see Ubachs, W. 270 (2001) 215
Verma, R., see Pandey, J.D. 270 (2001) 429

Volpp, H.-R., see Park, M.S. 270 (2001) 133
Wahlström, C.-G., see Ubachs, W. 270 (2001) 215
Wang, L., see Hua, X. 270 (2001) 93
Wang, Y., see Dong, S. 270 (2001) 309
Wei, J., S. Zhuo and G. Ju, Rapid estimation of the electronic correlation energies for van der Waals complexes 270 (2001) 31
Wolfe, S., see Tixier, S. 270 (2001) 263

Xie, D., Y. Lu, D. Xu and G. Yan, Theoretical studies on the potential energy surface and rovibrational states for the electronic ground state of carbonyl sulfide 270 (2001) 415
Xu, D., see Xie, D. 270 (2001) 415

Yamamoto, N., see Iwahashi, K. 270 (2001) 333
Yan, G., see Xie, D. 270 (2001) 415
Yekeler, H., An investigation of keto–enol tautomerism in *N*-vinyl-2-, and 3-pyrrolidinones using ab initio and density functional theory calculations 270 (2001) 391

Zhao, Q., see Piuzzi, F. 270 (2001) 205
Zheng, Y., see Brion, C.E. 270 (2001) 13
Zheng, Y., see Tixier, S. 270 (2001) 263
Zhuo, S., see Wei, J. 270 (2001) 31
Zimmer, M., see Chen, M.C. 270 (2001) 157

ELSEVIER

Chemical Physics 270 (2001) 489–500

Chemical Physics

www.elsevier.com/locate/chemphys

# Subject Index

## Methods and constructs

### Theoretical

*Computational methods for electronic structure*

Understanding the solvatochromism of 10-hydroxybenzo[h]quinoline. An appraisal of a polarity calibrator, J. Carlos del Valle and J. Catalán 270 (2001) 1

Theoretical investigation of the role of π–π interactions for the stability of phenylene ethynylene aggregates, M. Pickholz and S. Stafström 270 (2001) 245

Electron densities for the outer valence orbitals of pyridine: comparison of EMS measurements with near Hartree–Fock limit and density functional theory calculations, S. Tixier, W.A. Shapley, Y. Zheng, D.P. Chong, C.E. Brion, Z. Shi and S. Wolfe 270 (2001) 263

An investigation of keto–enol tautomerism in *N*-vinyl-2-, and 3-pyrrolidinones using ab initio and density functional theory calculations, H. Yekeler 270 (2001) 391

*-CI and valence bond approach*

Imaging of orbital electron densities by electron momentum spectroscopy – a chemical interpretation of the binary (e,2e) reaction, C.E. Brion, G. Cooper, Y. Zheng, I.V. Litvinyuk and I.E. McCarthy 270 (2001) 13

On the size extensivity of second-order Møller–Plesset perturbation theory based on a perfectly-paired generalized valence bond reference wavefunction, M. Sejpal and R.P. Messmer 270 (2001) 237

*-perturbative and many body approaches*

Rapid estimation of the electronic correlation energies for van der Waals complexes, J. Wei, S. Zhuo and G. Ju 270 (2001) 31

Second-order Møller–Plesset perturbation theory for computing molecular-field splitting: application to the $S2p_{3/2}$ level in $C_2H_{2n+1}SF_5$, $n = 0$, 1, and 2, T. Karlsen, K.J. Børve and L.J. Sæthre 270 (2001) 55

On the size extensivity of second-order Møller–Plesset perturbation theory based on a perfectly-paired generalized valence bond reference wavefunction, M. Sejpal and R.P. Messmer 270 (2001) 237

PII: S0301-0104(01)00436-0

Theoretical investigation of the role of π–π interactions for the stability of phenylene ethynylene aggregates, M. Pickholz and S. Stafström 270 (2001) 245

*-density functional theory*

Imaging of orbital electron densities by electron momentum spectroscopy – a chemical interpretation of the binary (e,2e) reaction, C.E. Brion, G. Cooper, Y. Zheng, I.V. Litvinyuk and I.E. McCarthy 270 (2001) 13

Excited electronic states and effect of vibronic-spin–orbit coupling on the radiative deactivation of the lowest triplet states of dioxins, E.A. Gastilovich, V.G. Klimenko, N.V. Korol'kova and G. Rauhut 270 (2001) 41

Tautomerism, hydrogen bonding and vibrational properties of 4-acetyl-3(5)-amino-5(3)-methylpyrazole, A. Szabó, V.I. Češljević and A. Kovács 270 (2001) 67

On the structure and spectroscopic properties of free and protonated adamanzanes, V. Galasso 270 (2001) 79

"Plasma" effect in the formation of long lifetime Rydberg states, X. Hua, J. Bai and L. Wang 270 (2001) 93

Theoretical investigation on $BaTiO_3$ with periodic density functional theory BLYP method, Z.-X. Chen, C.-G. Liu, Y. Chen and Y.-S. Jiang 270 (2001) 253

An investigation of keto–enol tautomerism in *N*-vinyl-2-, and 3-pyrrolidinones using ab initio and density functional theory calculations, H. Yekeler 270 (2001) 391

Sulfur in different chemical surroundings – S K XANES spectra of sulfur-containing heterocycles and their quantum-chemically supported interpretation, B. Flemmig, H. Modrow, K.H. Hallmeier, J. Hormes, J. Reinhold and R. Szargan 270 (2001) 405

*Semiempirical methods*

Excited electronic states and effect of vibronic-spin–orbit coupling on the radiative deactivation of the lowest triplet states of dioxins, E.A. Gastilovich, V.G. Klimenko, N.V. Korol'kova and G. Rauhut 270 (2001) 41

Bifluorophors: molecular design and excitation energy transfer mechanism, I.A. Ronova, A.Yu. Kovalevsky, S.A. Siling, S.V. Shamshin, A.V. Grachev and O.Yu. Tsyganova 270 (2001) 99

Structure and vibrational spectroscopy of halide ion hydrates: a study based on genetic algorithm, P. Chaudhury, R. Saha and S.P. Bhattacharyya 270 (2001) 277

*Algebraic approaches*

Computational aspects of motional symmetry in nuclear magnetic resonance spectroscopy, J.H. Kristensen and I. Farnan 270 (2001) 109

*Wavefunctions for highly excited and unbound states*

Second-order Møller–Plesset perturbation theory for computing molecular-field splitting: application to the $S2p_{3/2}$ level in $C_2H_{2n+1}SF_5$, $n = 0$, 1, and 2, T. Karlsen, K.J. Børve and L.J. Sæthre 270 (2001) 55

Theoretical studies on the potential energy surface and rovibrational states for the electronic ground state of carbonyl sulfide, D. Xie, Y. Lu, D. Xu and G. Yan 270 (2001) 415

*Spin states and magnetic interactions*

Computational aspects of motional symmetry in nuclear magnetic resonance spectroscopy, J.H. Kristensen and I. Farnan 270 (2001) 109

*Collisional and reactive molecular dynamics with non-frictional forces*
On the capture cross-section for charge neutralization, recombination, photoassociation and other barrierless reactions, R.D. Levine 270 (2001) 129

*Reactive molecular dynamics including dissipative processes*
The dynamics of oxygen atom formation in the UV photodissociation of nitromethane, M.S. Park, K.-H. Jung, H.P. Upadhyaya and H.-R. Volpp 270 (2001) 133

*Intramolecular dynamics*
Theoretical studies on the potential energy surface and rovibrational states for the electronic ground state of carbonyl sulfide, D. Xie, Y. Lu, D. Xu and G. Yan 270 (2001) 415

*Molecular dynamics of many particle systems and condensed phases*
Nonstandard reaction kinetics: microscopic simulations of system with product removal, B. Nowakowski, A. Lemarchand and E. Nowakowska 270 (2001) 287

*Quasiparticle dynamics (incl. excitons, polarons)*
Towards proper parametrization in the exciton transfer and relaxation problem: dimer, V. Čápek, I. Barvík and P. Heřman 270 (2001) 141

*Statistical computational methods (incl. Monte Carlo)*
Photoisomerization of green fluorescent protein and the dimensions of the chromophore cavity, M.C. Chen, C.R. Lambert, J.D. Urgitis and M. Zimmer 270 (2001) 157
Nonstandard reaction kinetics: microscopic simulations of system with product removal, B. Nowakowski, A. Lemarchand and E. Nowakowska 270 (2001) 287

*Dynamics of structures, lattices and macromolecular conformations*
Photoisomerization of green fluorescent protein and the dimensions of the chromophore cavity, M.C. Chen, C.R. Lambert, J.D. Urgitis and M. Zimmer 270 (2001) 157
Electronic structure and chemical stabilization of $C_{28}$ fullerene, Yu.N. Makurin, A.A. Sofronov, A.I. Gusev and A.L. Ivanovsky 270 (2001) 293
Potential lattice dynamical simulations of ice, S. Dong, Y. Wang and J. Li 270 (2001) 309

*Non-equilibrium statistical mechanics*
Towards proper parametrization in the exciton transfer and relaxation problem: dimer, V. Čápek, I. Barvík and P. Heřman 270 (2001) 141
Third-order transport properties of ions in electrostatic fields, A.D. Koutselos 270 (2001) 165
Inversion of the Kirkwood–Buff theory of solutions: application to binary systems, J.D. Pandey and R. Verma 270 (2001) 429
Non-equilibrium vibrational kinetics and 'hot atom' models in the recombination of hydrogen atoms on surfaces, E. Molinari and M. Tomellini 270 (2001) 439

*Non-equilibrium thermodynamic and hydrodynamic theories*
On the simplified state-to-state transport coefficients, E.V. Kustova 270 (2001) 177
On the accuracy of non-equilibrium transport coefficients calculation, E.V. Kustova, E.A. Nagnibeda and A. Chikhaoui 270 (2001) 459

*Equilibrium statistical mechanics and thermodynamics*
Orientation correlation of neopentane molecules in liquid state through available diffraction data, S. Sarkar, P.P. Nath and R.N. Joarder 270 (2001) 197

**Experiment**

*Molecular spectroscopy*
Understanding the solvatochromism of 10-hydroxybenzo[h]quinoline. An appraisal of a polarity calibrator, J. Carlos del Valle and J. Catalán 270 (2001) 1
Bifluorophors: molecular design and excitation energy transfer mechanism, I.A. Ronova, A.Yu. Kovalevsky, S.A. Siling, S.V. Shamshin, A.V. Grachev and O.Yu. Tsyganova 270 (2001) 99
On the capture cross-section for charge neutralization, recombination, photoassociation and other barrierless reactions, R.D. Levine 270 (2001) 129

*-infrared*
Tautomerism, hydrogen bonding and vibrational properties of 4-acetyl-3(5)-amino-5(3)-methylpyrazole, A. Szabó, V.I. Češljević and A. Kovács 270 (2001) 67

*-UV*
Ultraviolet spectroscopy and tautomerism of the DNA base guanine and its hydrate formed in a supersonic jet, F. Piuzzi, M. Mons, I. Dimicoli, B. Tardivel and Q. Zhao 270 (2001) 205
Lifetime measurements on the $c_4'^1\Sigma_u^+$, $v = 0$, 1 and 2 states of molecular nitrogen, W. Ubachs, R. Lang, I. Velchev, W.-Ü.L. Tchang-Brillet, A. Johansson, Z.S. Li, V. Lokhnygin and C.-G. Wahlström 270 (2001) 215

*-visible*
Excited electronic states and effect of vibronic-spin–orbit coupling on the radiative deactivation of the lowest triplet states of dioxins, E.A. Gastilovich, V.G. Klimenko, N.V. Korol'kova and G. Rauhut 270 (2001) 41

*Photoelectron and Auger spectroscopy*
Second-order Møller–Plesset perturbation theory for computing molecular-field splitting: application to the $S2p_{3/2}$ level in $C_2H_{2n+1}SF_5$, $n = 0$, 1, and 2, T. Karlsen, K.J. Børve and L.J. Sæthre 270 (2001) 55
On the structure and spectroscopic properties of free and protonated adamanzanes, V. Galasso 270 (2001) 79

*Multiphoton ionization*
The dynamics of oxygen atom formation in the UV photodissociation of nitromethane, M.S. Park, K.-H. Jung, H.P. Upadhyaya and H.-R. Volpp 270 (2001) 133

*X-ray spectroscopy*
Sulfur in different chemical surroundings – S K XANES spectra of sulfur-containing heterocycles and their quantum-chemically supported interpretation, B. Flemmig, H. Modrow, K.H. Hallmeier, J. Hormes, J. Reinhold and R. Szargan 270 (2001) 405

*Electron impact spectroscopy*
Imaging of orbital electron densities by electron momentum spectroscopy – a chemical interpretation of the binary (e,2e) reaction, C.E. Brion, G. Cooper, Y. Zheng, I.V. Litvinyuk and I.E. McCarthy 270 (2001) 13
Electron densities for the outer valence orbitals of pyridine: comparison of EMS measurements with near Hartree–Fock limit and density functional theory calculations, S. Tixier, W.A. Shapley, Y. Zheng, D.P. Chong, C.E. Brion, Z. Shi and S. Wolfe 270 (2001) 263
Ionic photofragmentation and photoionization of dimethyl ether in the VUV and soft X-ray regions (8.5–80 eV) – absolute oscillator strengths for molecular and dissociative photoionization, R. Feng, G. Cooper and C.E. Brion 270 (2001) 319
Ejection of cluster ions as a result of electron impact ionization of argon clusters, A.V. Malakhovskii 270 (2001) 471

*Laser induced fluorescence*
Dispersed fluorescence spectra of chlorobenzene, P. Imhof and K. Kleinermanns 270 (2001) 227
Hole-burning spectra of tropolone–$(CO_2)_n$ ($n = 1, 2$) van der Waals complexes and density functional study, K. Iwahashi, N. Yamamoto, T. Fukuchi, J. Furusawa and H. Sekiya 270 (2001) 333
Fluorescence of $UO_2^{2+}$ in a non-complexing medium: $HClO_4/NaClO_4$ up to 10 M, I. Billard, A. Rustenholtz, L. Sémon and K. Lützenkirchen 270 (2001) 345

*Ultrafast measurements*
Towards proper parametrization in the exciton transfer and relaxation problem: dimer, V. Čápek, I. Barvík and P. Heřman 270 (2001) 141

*Synchrotron spectroscopies*
Observation of photon cascade emission in the $Pr^{3+}$-doped perovskite $KMgF_3$, I. Sokólska and S. Kück 270 (2001) 355
A study of the threshold photoelectron spectra and the photoionisation yield curves of the silicon tetrahalides, L. Cooper, L.G. Shpinkova, D.M.P. Holland and D.A. Shaw 270 (2001) 363
Sulfur in different chemical surroundings – S K XANES spectra of sulfur-containing heterocycles and their quantum-chemically supported interpretation, B. Flemmig, H. Modrow, K.H. Hallmeier, J. Hormes, J. Reinhold and R. Szargan 270 (2001) 405

*Optoacoustic spectroscopy*
Bulk rotational relaxation time and cross-section in gas mixtures, M. Terzić, D. Markushev and J. Jovanović-Kurepa 270 (2001) 383

*Mass spectroscopy*
"Plasma" effect in the formation of long lifetime Rydberg states, X. Hua, J. Bai and L. Wang 270 (2001) 93
A study of the threshold photoelectron spectra and the photoionisation yield curves of the silicon tetrahalides, L. Cooper, L.G. Shpinkova, D.M.P. Holland and D.A. Shaw 270 (2001) 363

*X-ray, electron and neutron diffraction*
Orientation correlation of neopentane molecules in liquid state through available diffraction data, S. Sarkar, P.P. Nath and R.N. Joarder 270 (2001) 197

*Neutron scattering (inelastic and quasielastic)*
Potential lattice dynamical simulations of ice, S. Dong, Y. Wang and J. Li 270 (2001) 309

## Objects

### Bulk systems

*Gases*
The dynamics of oxygen atom formation in the UV photodissociation of nitromethane, M.S. Park, K.-H. Jung, H.P. Upadhyaya and H.-R. Volpp 270 (2001) 133
Third-order transport properties of ions in electrostatic fields, A.D. Koutselos 270 (2001) 165
On the simplified state-to-state transport coefficients, E.V. Kustova 270 (2001) 177
Nonstandard reaction kinetics: microscopic simulations of system with product removal, B. Nowakowski, A. Lemarchand and E. Nowakowska 270 (2001) 287
On the accuracy of non-equilibrium transport coefficients calculation, E.V. Kustova, E.A. Nagnibeda and A. Chikhaoui 270 (2001) 459

*Supersonic beams*
Ultraviolet spectroscopy and tautomerism of the DNA base guanine and its hydrate formed in a supersonic jet, F. Piuzzi, M. Mons, I. Dimicoli, B. Tardivel and Q. Zhao 270 (2001) 205
Dispersed fluorescence spectra of chlorobenzene, P. Imhof and K. Kleinermanns 270 (2001) 227
Hole-burning spectra of tropolone–$(CO_2)_n$ ($n = 1, 2$) van der Waals complexes and density functional study, K. Iwahashi, N. Yamamoto, T. Fukuchi, J. Furusawa and H. Sekiya 270 (2001) 333

*Liquid mixtures and solutions*
Understanding the solvatochromism of 10-hydroxybenzo[h]quinoline. An appraisal of a polarity calibrator, J. Carlos del Valle and J. Catalán 270 (2001) 1
Fluorescence of $UO_2^{2+}$ in a non-complexing medium: $HClO_4/NaClO_4$ up to 10 M, I. Billard, A. Rustenholtz, L. Sémon and K. Lützenkirchen 270 (2001) 345
Inversion of the Kirkwood–Buff theory of solutions: application to binary systems, J.D. Pandey and R. Verma 270 (2001) 429

*Crystals*
Towards proper parametrization in the exciton transfer and relaxation problem: dimer, V. Čápek, I. Barvík and P. Heřman 270 (2001) 141
Theoretical investigation on $BaTiO_3$ with periodic density functional theory BLYP method, Z.-X. Chen, C.-G. Liu, Y. Chen and Y.-S. Jiang 270 (2001) 253
Potential lattice dynamical simulations of ice, S. Dong, Y. Wang and J. Li 270 (2001) 309
Observation of photon cascade emission in the $Pr^{3+}$-doped perovskite $KMgF_3$, I. Sokólska and S. Kück 270 (2001) 355

*Complex fluids*
Orientation correlation of neopentane molecules in liquid state through available diffraction data, S. Sarkar, P.P. Nath and R.N. Joarder 270 (2001) 197

*Polymers*
Bifluorophors: molecular design and excitation energy transfer mechanism, I.A. Ronova, A.Yu. Kovalevsky, S.A. Siling, S.V. Shamshin, A.V. Grachev and O.Yu. Tsyganova 270 (2001) 99
Theoretical investigation of the role of π–π interactions for the stability of phenylene ethynylene aggregates, M. Pickholz and S. Stafström 270 (2001) 245
An investigation of keto–enol tautomerism in *N*-vinyl-2-, and 3-pyrrolidinones using ab initio and density functional theory calculations, H. Yekeler 270 (2001) 391

*Surfaces*
Non-equilibrium vibrational kinetics and 'hot atom' models in the recombination of hydrogen atoms on surfaces, E. Molinari and M. Tomellini 270 (2001) 439

*Plasmas*
"Plasma" effect in the formation of long lifetime Rydberg states, X. Hua, J. Bai and L. Wang 270 (2001) 93
Third-order transport properties of ions in electrostatic fields, A.D. Koutselos 270 (2001) 165

**Microscopic and mesoscopic systems**

*Single atoms, molecules and assemblies (incl. biological)*
Ultraviolet spectroscopy and tautomerism of the DNA base guanine and its hydrate formed in a supersonic jet, F. Piuzzi, M. Mons, I. Dimicoli, B. Tardivel and Q. Zhao 270 (2001) 205
An investigation of keto–enol tautomerism in *N*-vinyl-2-, and 3-pyrrolidinones using ab initio and density functional theory calculations, H. Yekeler 270 (2001) 391

*Molecules (neutral and ionic)*
Bifluorophors: molecular design and excitation energy transfer mechanism, I.A. Ronova, A.Yu. Kovalevsky, S.A. Siling, S.V. Shamshin, A.V. Grachev and O.Yu. Tsyganova 270 (2001) 99
Sulfur in different chemical surroundings – S K XANES spectra of sulfur-containing heterocycles and their quantum-chemically supported interpretation, B. Flemmig, H. Modrow, K.H. Hallmeier, J. Hormes, J. Reinhold and R. Szargan 270 (2001) 405

*-diatomic*
On the simplified state-to-state transport coefficients, E.V. Kustova 270 (2001) 177
Lifetime measurements on the $c_4'^1\Sigma_u^+$, $v = 0$, 1 and 2 states of molecular nitrogen, W. Ubachs, R. Lang, I. Velchev, W.-Ü.L. Tchang-Brillet, A. Johansson, Z.S. Li, V. Lokhnygin and C.-G. Wahlström 270 (2001) 215
On the accuracy of non-equilibrium transport coefficients calculation, E.V. Kustova, E.A. Nagnibeda and A. Chikhaoui 270 (2001) 459

*-small polyatomics*
Imaging of orbital electron densities by electron momentum spectroscopy – a chemical interpretation of the binary (e,2e) reaction, C.E. Brion, G. Cooper, Y. Zheng, I.V. Litvinyuk and I.E. McCarthy 270 (2001) 13

Second-order Møller–Plesset perturbation theory for computing molecular-field splitting: application to the $S2p_{3/2}$ level in $C_2H_{2n+1}SF_5$, $n = 0$, 1, and 2, T. Karlsen, K.J. Børve and L.J. Sæthre 270 (2001) 55
Tautomerism, hydrogen bonding and vibrational properties of 4-acetyl-3(5)-amino-5(3)-methylpyrazole, A. Szabó, V.I. Češljević and A. Kovács 270 (2001) 67
Ionic photofragmentation and photoionization of dimethyl ether in the VUV and soft X-ray regions (8.5–80 eV) – absolute oscillator strengths for molecular and dissociative photoionization, R. Feng, G. Cooper and C.E. Brion 270 (2001) 319
A stu dy of the threshold photoelectron spectra and the photoionisation yield curves of the silicon tetrahalides, L. Cooper, L.G. Shpinkova, D.M.P. Holland and D.A. Shaw 270 (2001) 363
Theoretical studies on the potential energy surface and rovibrational states for the electronic ground state of carbonyl sulfide, D. Xie, Y. Lu, D. Xu and G. Yan 270 (2001) 415

*-aromatics*
Dispersed fluorescence spectra of chlorobenzene, P. Imhof and K. Kleinermanns 270 (2001) 227
Electron densities for the outer valence orbitals of pyridine: comparison of EMS measurements with near Hartree–Fock limit and density functional theory calculations, S. Tixier, W.A. Shapley, Y. Zheng, D.P. Chong, C.E. Brion, Z. Shi and S. Wolfe 270 (2001) 263

*-other large*
Excited electronic states and effect of vibronic-spin–orbit coupling on the radiative deactivation of the lowest triplet states of dioxins, E.A. Gastilovich, V.G. Klimenko, N.V. Korol'kova and G. Rauhut 270 (2001) 41
On the structure and spectroscopic properties of free and protonated adamanzanes, V. Galasso 270 (2001) 79
Electronic structure and chemical stabilization of $C_{28}$ fullerene, Yu.N. Makurin, A.A. Sofronov, A.I. Gusev and A.L. Ivanovsky 270 (2001) 293

*Molecular aggregates*
On the size extensivity of second-order Møller–Plesset perturbation theory based on a perfectly-paired generalized valence bond reference wavefunction, M. Sejpal and R.P. Messmer 270 (2001) 237
Structure and vibrational spectroscopy of halide ion hydrates: a study based on genetic algorithm, P. Chaudhury, R. Saha and S.P. Bhattacharyya 270 (2001) 277

*-van der Waals molecules*
Rapid estimation of the electronic correlation energies for van der Waals complexes, J. Wei, S. Zhuo and G. Ju 270 (2001) 31
Hole-burning spectra of tropolone–$(CO_2)_n$ ($n = 1, 2$) van der Waals complexes and density functional study, K. Iwahashi, N. Yamamoto, T. Fukuchi, J. Furusawa and H. Sekiya 270 (2001) 333

*-clusters*
Structure and vibrational spectroscopy of halide ion hydrates: a study based on genetic algorithm, P. Chaudhury, R. Saha and S.P. Bhattacharyya 270 (2001) 277
Potential lattice dynamical simulations of ice, S. Dong, Y. Wang and J. Li 270 (2001) 309

Ejection of cluster ions as a result of electron impact ionization of argon clusters, A.V. Malakhovskii 270 (2001) 471

*Quasiparticles (incl. excitons)*
Towards proper parametrization in the exciton transfer and relaxation problem: dimer, V. Čápek, I. Barvík and P. Heřman 270 (2001) 141

*Proteins*
Photoisomerization of green fluorescent protein and the dimensions of the chromophore cavity, M.C. Chen, C.R. Lambert, J.D. Urgitis and M. Zimmer 270 (2001) 157

## Phenomena

*Molecular structure*
Rapid estimation of the electronic correlation energies for van der Waals complexes, J. Wei, S. Zhuo and G. Ju 270 (2001) 31
Tautomerism, hydrogen bonding and vibrational properties of 4-acetyl-3(5)-amino-5(3)-methylpyrazole, A. Szabó, V.I. Češljević and A. Kovács 270 (2001) 67
On the structure and spectroscopic properties of free and protonated adamanzanes, V. Galasso 270 (2001) 79
Orientation correlation of neopentane molecules in liquid state through available diffraction data, S. Sarkar, P.P. Nath and R.N. Joarder 270 (2001) 197
Theoretical investigation of the role of π–π interactions for the stability of phenylene ethynylene aggregates, M. Pickholz and S. Stafström 270 (2001) 245
Structure and vibrational spectroscopy of halide ion hydrates: a study based on genetic algorithm, P. Chaudhury, R. Saha and S.P. Bhattacharyya 270 (2001) 277
Hole-burning spectra of tropolone–$(CO_2)_n$ ($n = 1, 2$) van der Waals complexes and density functional study, K. Iwahashi, N. Yamamoto, T. Fukuchi, J. Furusawa and H. Sekiya 270 (2001) 333
An investigation of keto–enol tautomerism in *N*-vinyl-2-, and 3-pyrrolidinones using ab initio and density functional theory calculations, H. Yekeler 270 (2001) 391

*Vibrations and rotations of molecules*
Tautomerism, hydrogen bonding and vibrational properties of 4-acetyl-3(5)-amino-5(3)-methylpyrazole, A. Szabó, V.I. Češljević and A. Kovács 270 (2001) 67
Dispersed fluorescence spectra of chlorobenzene, P. Imhof and K. Kleinermanns 270 (2001) 227
Structure and vibrational spectroscopy of halide ion hydrates: a study based on genetic algorithm, P. Chaudhury, R. Saha and S.P. Bhattacharyya 270 (2001) 277
Theoretical studies on the potential energy surface and rovibrational states for the electronic ground state of carbonyl sulfide, D. Xie, Y. Lu, D. Xu and G. Yan 270 (2001) 415

*Electronic structure and states*
Imaging of orbital electron densities by electron momentum spectroscopy – a chemical interpretation of the binary (e,2e) reaction, C.E. Brion, G. Cooper, Y. Zheng, I.V. Litvinyuk and I.E. McCarthy 270 (2001) 13

Second-order Møller–Plesset perturbation theory for computing molecular-field splitting: application to the $S2p_{3/2}$ level in $C_2H_{2n+1}SF_5$, $n = 0$, 1, and 2, T. Karlsen, K.J. Børve and L.J. Sæthre 270 (2001) 55
Photoisomerization of green fluorescent protein and the dimensions of the chromophore cavity, M.C. Chen, C.R. Lambert, J.D. Urgitis and M. Zimmer 270 (2001) 157
Ultraviolet spectroscopy and tautomerism of the DNA base guanine and its hydrate formed in a supersonic jet, F. Piuzzi, M. Mons, I. Dimicoli, B. Tardivel and Q. Zhao 270 (2001) 205
Theoretical investigation on $BaTiO_3$ with periodic density functional theory BLYP method, Z.-X. Chen, C.-G. Liu, Y. Chen and Y.-S. Jiang 270 (2001) 253
Electron densities for the outer valence orbitals of pyridine: comparison of EMS measurements with near Hartree–Fock limit and density functional theory calculations, S. Tixier, W.A. Shapley, Y. Zheng, D.P. Chong, C.E. Brion, Z. Shi and S. Wolfe 270 (2001) 263
Electronic structure and chemical stabilization of $C_{28}$ fullerene, Yu.N. Makurin, A.A. Sofronov, A.I. Gusev and A.L. Ivanovsky 270 (2001) 293
Observation of photon cascade emission in the $Pr^{3+}$-doped perovskite $KMgF_3$, I. Sokólska and S. Kück 270 (2001) 355
Sulfur in different chemical surroundings – S K XANES spectra of sulfur-containing heterocycles and their quantum-chemically supported interpretation, B. Flemmig, H. Modrow, K.H. Hallmeier, J. Hormes, J. Reinhold and R. Szargan 270 (2001) 405

*Electric and magnetic properties*
On the structure and spectroscopic properties of free and protonated adamanzanes, V. Galasso 270 (2001) 79

*Molecular interactions*
Rapid estimation of the electronic correlation energies for van der Waals complexes, J. Wei, S. Zhuo and G. Ju 270 (2001) 31
On the capture cross-section for charge neutralization, recombination, photoassociation and other barrierless reactions, R.D. Levine 270 (2001) 129
On the size extensivity of second-order Møller–Plesset perturbation theory based on a perfectly-paired generalized valence bond reference wavefunction, M. Sejpal and R.P. Messmer 270 (2001) 237
Hole-burning spectra of tropolone–$(CO_2)_n$ ($n = 1, 2$) van der Waals complexes and density functional study, K. Iwahashi, N. Yamamoto, T. Fukuchi, J. Furusawa and H. Sekiya 270 (2001) 333

*Spectral bandshapes and intensities*
Ionic photofragmentation and photoionization of dimethyl ether in the VUV and soft X-ray regions (8.5–80 eV) – absolute oscillator strengths for molecular and dissociative photoionization, R. Feng, G. Cooper and C.E. Brion 270 (2001) 319

*Energy transfer processes*
Bifluorophors: molecular design and excitation energy transfer mechanism, I.A. Ronova, A.Yu. Kovalevsky, S.A. Siling, S.V. Shamshin, A.V. Grachev and O.Yu. Tsyganova 270 (2001) 99

Fluorescence of $UO_2^{2+}$ in a non-complexing medium: $HClO_4/NaClO_4$ up to 10 M, I. Billard, A. Rustenholtz, L. Sémon and K. Lützenkirchen 270 (2001) 345
Bulk rotational relaxation time and cross-section in gas mixtures, M. Terzić, D. Markushev and J. Jovanović-Kurepa 270 (2001) 383

*Molecular photophysical processes*
Understanding the solvatochromism of 10-hydroxybenzo[h]quinoline. An appraisal of a polarity calibrator, J. Carlos del Valle and J. Catalán 270 (2001) 1
Excited electronic states and effect of vibronic-spin–orbit coupling on the radiative deactivation of the lowest triplet states of dioxins, E.A. Gastilovich, V.G. Klimenko, N.V. Korol'kova and G. Rauhut 270 (2001) 41
Lifetime measurements on the $c_4'^1\Sigma_u^+$, $v = 0$, 1 and 2 states of molecular nitrogen, W. Ubachs, R. Lang, I. Velchev, W.-Ü.L. Tchang-Brillet, A. Johansson, Z.S. Li, V. Lokhnygin and C.-G. Wahlström 270 (2001) 215
Ionic photofragmentation and photoionization of dimethyl ether in the VUV and soft X-ray regions (8.5–80 eV) – absolute oscillator strengths for molecular and dissociative photoionization, R. Feng, G. Cooper and C.E. Brion 270 (2001) 319
A study of the threshold photoelectron spectra and the photoionisation yield curves of the silicon tetrahalides, L. Cooper, L.G. Shpinkova, D.M.P. Holland and D.A. Shaw 270 (2001) 363
Bulk rotational relaxation time and cross-section in gas mixtures, M. Terzić, D. Markushev and J. Jovanović-Kurepa 270 (2001) 383

*Photochemistry*
The dynamics of oxygen atom formation in the UV photodissociation of nitromethane, M.S. Park, K.-H. Jung, H.P. Upadhyaya and H.-R. Volpp 270 (2001) 133

*Intramolecular dynamics*
On the capture cross-section for charge neutralization, recombination, photoassociation and other barrierless reactions, R.D. Levine 270 (2001) 129

*-vibrational energy redistribution (incl. vibrational dissociation)*
On the simplified state-to-state transport coefficients, E.V. Kustova 270 (2001) 177

*Luminescence spectra, yields and lifetimes*
Fluorescence of $UO_2^{2+}$ in a non-complexing medium: $HClO_4/NaClO_4$ up to 10 M, I. Billard, A. Rustenholtz, L. Sémon and K. Lützenkirchen 270 (2001) 345
Observation of photon cascade emission in the $Pr^{3+}$-doped perovskite $KMgF_3$, I. Sokólska and S. Kück 270 (2001) 355

*Multiphoton phenomena*
Bulk rotational relaxation time and cross-section in gas mixtures, M. Terzić, D. Markushev and J. Jovanović-Kurepa 270 (2001) 383

*Reactions (incl. dissociation)*
On the capture cross-section for charge neutralization, recombination, photoassociation and other barrierless reactions, R.D. Levine 270 (2001) 129

*-collisional*
Nonstandard reaction kinetics: microscopic simulations of system with product removal, B. Nowakowski, A. Lemarchand and E. Nowakowska 270 (2001) 287

*Proton and hydrogen atom transfer*
Understanding the solvatochromism of 10-hydroxybenzo[h]quinoline. An appraisal of a polarity calibrator, J. Carlos del Valle and J. Catalán 270 (2001) 1

*Ionization (incl. Rydberg states)*
"Plasma" effect in the formation of long lifetime Rydberg states, X. Hua, J. Bai and L. Wang 270 (2001) 93
A study of the threshold photoelectron spectra and the photoionisation yield curves of the silicon tetrahalides, L. Cooper, L.G. Shpinkova, D.M.P. Holland and D.A. Shaw 270 (2001) 363

*Molecular motion (incl. diffusive)*
Computational aspects of motional symmetry in nuclear magnetic resonance spectroscopy, J.H. Kristensen and I. Farnan 270 (2001) 109
Third-order transport properties of ions in electrostatic fields, A.D. Koutselos 270 (2001) 165

*Surface chemical physics*
Non-equilibrium vibrational kinetics and 'hot atom' models in the recombination of hydrogen atoms on surfaces, E. Molinari and M. Tomellini 270 (2001) 439

*-surface reactions*
Non-equilibrium vibrational kinetics and 'hot atom' models in the recombination of hydrogen atoms on surfaces, E. Molinari and M. Tomellini 270 (2001) 439

*-catalysis*
Non-equilibrium vibrational kinetics and 'hot atom' models in the recombination of hydrogen atoms on surfaces, E. Molinari and M. Tomellini 270 (2001) 439

*Thermodynamic and transport properties*
Third-order transport properties of ions in electrostatic fields, A.D. Koutselos 270 (2001) 165
On the simplified state-to-state transport coefficients, E.V. Kustova 270 (2001) 177
On the accuracy of non-equilibrium transport coefficients calculation, E.V. Kustova, E.A. Nagnibeda and A. Chikhaoui 270 (2001) 459

*Structure of solids, liquids and gases*
Orientation correlation of neopentane molecules in liquid state through available diffraction data, S. Sarkar, P.P. Nath and R.N. Joarder 270 (2001) 197

*Molecular self-assembly and -organization*
Theoretical investigation of the role of $\pi$–$\pi$ interactions for the stability of phenylene ethynylene aggregates, M. Pickholz and S. Stafström 270 (2001) 245